SPECIAL PROJECT PROGRESS REPORT

Progress Reports should be 2 to 10 pages in length, depending on importance of the project. All the following mandatory information needs to be provided.

Reporting year	2015/16
Project Title:	Global atmospheric chemistry modelling
Computer Project Account:	spdeacm
Principal Investigator(s):	O. Stein, M.G. Schultz
Affiliation:	Research Center Juelich
Name of ECMWF scientist(s) collaborating to the project (if applicable)	J. Flemming, A. Inness, L. Jones, R. Engelen
Start date of the project:	2014
Expected end date:	2017

Computer resources allocated/used for the current year and the previous one

(if applicable)

Please answer for all project resources

		Previous year		Current year	
		Allocated	Used	Allocated	Used
High Performance Computing Facility	(units)	950000	911180	600000	0
Data storage capacity	(Gbytes)	30000	47291	30000	47291

Summary of project objectives

(10 lines max)

- Development of a chemistry module for IFS (CIFS-MOZ)
- Maintenance and improvements of the quasi-operational coupled MACC system MOZ-IFS
- Evaluation of the MOZ-IFS and CIFS-MOZ model for the troposphere and stratosphere
- Evaluation of MACC NRT forecasts and reanalysis
- investigate global budgets of trace gases in the atmosphere
- scientific model development of gas-phase chemistry in MOZART3, MOZ-IFS and CIFS-MOZ
- development and processing of global emission inventories

Summary of problems encountered (if any)

Our group member in charge of CIFS-MOZ development left FZ Jülich by February 2016. Thus we decided to not pursue this development line any further and also to not take an active part in any CAMS activities. Therefore, other than expected, substantial HPC allocation is not needed anymore for 2016 and following years. Nevertheless, access to ecgate and storage capacity on ecfs will be needed for several reasons as explained in the extended report and in the continuation plan.

Summary of results of the current year (from July of previous year to June of current year)

See attached doc-file

List of publications/reports from the project with complete references

Peer-reviewed:

Eskes, H., Huijnen, V., Arola, A., Benedictow, A., Blechschmidt, A.-M., Botek, E., Boucher, O., Bouarar, I., Chabrillat, S., Cuevas, E., Engelen, R., Flentje, H., Gaudel, A., Griesfeller, J., Jones, L., Kapsomenakis, J., Katragkou, E., Kinne, S., Langerock, B., Razinger, M., Richter, A., Schultz, M., Schulz, M., Sudarchikova, N., Thouret, V., Vrekoussis, M., Wagner, A., and Zerefos, C.: Validation of reactive gases and aerosols in the MACC global analysis and forecast system, Geosci. Model Dev., 8, 3523-3543, doi:10.5194/gmd-8-3523-2015, 2015.

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For any publications prior to 2014 we refer to the references in the spdeacm final report 2012-2014.

Summary of plans for the continuation of the project

(10 lines max)

Work on the evaluation of MACC simulations has been finished with several recent publications. Nevertheless, various MACC and CAMS chemical atmospheric data as well as upcoming CAMS reanalysis will be constantly used for atmospheric science case studies and model evaluation. Moreover, our long-term obligation to host MACC and CAMS chemical boundary condition data for use in RAQ models makes it necessary to access the ecgate server and the ECMWF archives, also beyond 2017. More recently we started to use high-resolution operational analyses and reanalysis products to study volcanic eruptions and gravity waves. This activity will continue during the project. For the next two years, only rudimentary access to cca will be needed.

Global modelling of atmospheric chemistry
special project SPDEACM interim report
June 2016

Olaf Stein, Martin G. Schultz
Forschungszentrum Jülich

For SPDEACM 2015/2016 was a transition period between the EU project MACC-III (2012-2014) and the establishment of the Copernicus Atmospheric Monitoring System (CAMS) which, for the global reactive gases part, took effect in early 2016. In the meantime we tried to update and maintain the global model system CIFS-MOZ (IFS with integrated MOZART chemistry) with limited man-power. With the leaving of our group member Yi Heng in February 2016 we were not able to pursue this effort any further and stopped any C-IFS development. Currently, the SPDEACM accounts are heavily used for data transfer of meteorological and chemical data from the MARS and ECFS archives to the Jülich supercomputing systems. In an ongoing and long-term activity we provide chemical boundary conditions from the global CAMS forecasts to regional air quality modellers in NRT. Moreover, data from historic operational forecasts as well as meteorological and chemical reanalysis products are stored in Jülich for scientific analysis. A series of publications in peer-reviewed journals closely related to our activities within SPDEACM could be published during the last year.

C-IFS

In 2015, CIFS-MOZ (Stein and Flemming, 2015) was updated to IFS cycle 41R1 on the CRAY machine (cca). SPDEACM participated in two publications describing the CIFS system (Flemming et al., 2015; Inness et al., 2015). Our new group member Yi Heng achieved significant progress with CIFS-MOZ, the group's major development. After adapting to the new IFS version, we implemented an updated stratospheric chemical scheme. Several longer sensitivity simulations with CIFS in resolution T255 were performed, initially thought to be necessary for evaluation of the new stratospheric chemistry implementation. Unfortunately, Yi Heng left FZ Jülich in February 2016. Therefore we decided to shut down our CIFS developments and to cancel our planned activities for CAMS. As a consequence, no substantial computer allocation on cca will be needed for the years 2016/2017.

Data services supporting CAMS and MACC

As a long-term effort NRT data from the operational CAMS forecasts as well as from the GFAS fire emission inventory (Kaiser et al. 2012) are transferred to FZ Jülich on a daily basis and made available to the public via our OWS interface JOIN (Waychal et al. 2013; http://join.iek.fz-juelich.de/). In addition, we started to download all chemical species concentrations from the MACC reanalysis 2003-2012 which are not publically available from the MARS archive. Tracer fields from the CAMS operational forecasts and from the MACC reanalysis are used for scientific analysis of atmospheric chemistry (Gaudel et al., 2015; Lyapina et al, 2016; Kracher et al, 2016) and serve as boundary conditions for regional air quality models (Sheel et al., 2014; Liora et al., 2016). For the latter purpose, our existing Web Coverage Service (WCS) for sharing individually tailored model results is currently being re-engineered to make use of a modern, scalable database technology in order to improve performance, enhance flexibility, and allow the operation of catalogue services. The WCS protocol shall be upgraded to WCS2.0 and the metadata shall be interfaced with the EUDAT (https://www.eudat.eu/) service structure. In effect the current self-written WCS software package shall be replaced by a modernized and more efficient out-of-the-box solution (Schultz et al., 2016).

IFS-MOZ

Results from the coupled system IFS-MOZ run in MACC reanalysis and forecasts from 2010 to 2014 have been evaluated and analysed in several scientific papers which appeared in 2015/16. The publications of Lefever et al. (2015), Wagner et al. (2015), Katragkou et al. (2015) and Gaudel et al. (2015) have already been summarized in last year's report. Moreover, our paper on the reduction of the warming potential of nitrous oxide by an enhanced Brewer-Dobson circulation under climate change conditions was recently published (Kracher et al., 2016).

Eskes et al. (2015) evaluate reactive gases and aerosols in the MACC global analysis and forecast system simulated with IFS-MOZ during 2012-2014 (MACC o-suite). The paper discusses the approach to validation that has been developed by the MACC VAL group. Topics discussed are the validation requirements, the operational aspects, the measurement data sets used, the structure of the validation reports, the models and assimilation systems validated, the procedure to introduce new upgrades, and the scoring methods. Exemplarily shown here is validation of free tropospheric ozone with respect to combined surface and free tropospheric ozone observations from the GAW network, IAGOS aircraft data, and ozone sondes for different regions (Figure 1).

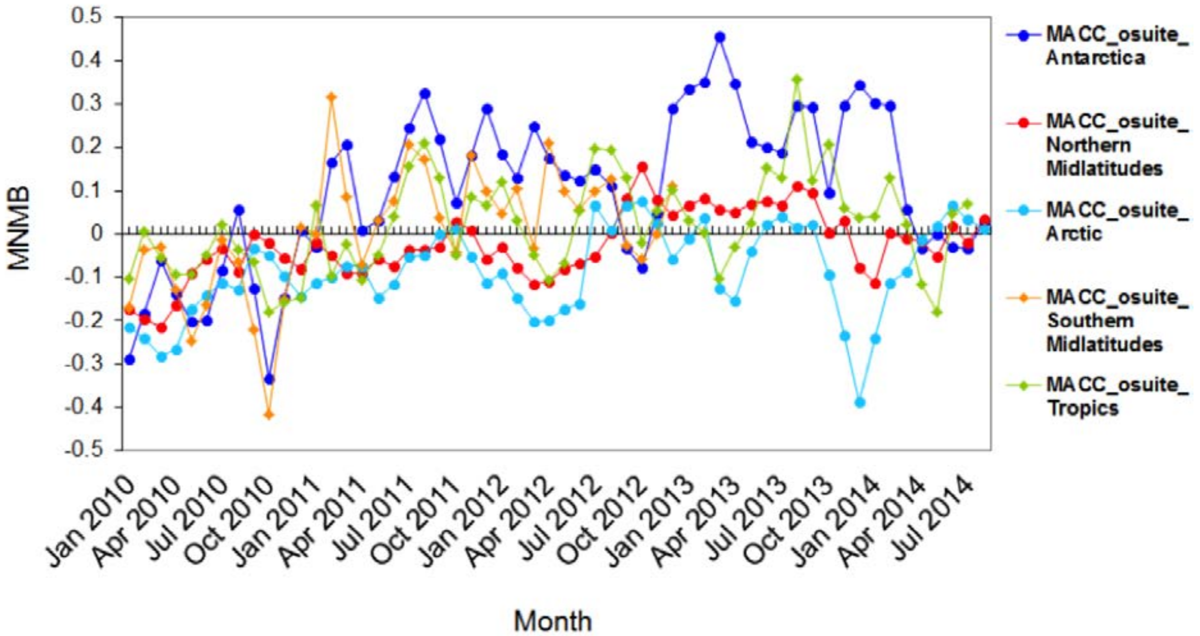

Figure 1: Modified normalized mean bias (MNMB) of ozone in the free troposphere (750–200 hPa) in the tropics and 750–300 hPa elsewhere) of MACC o-suite against aggregated sonde data in four different regions.

Liora et al. (2016) apply chemical boundary conditions from the MACC reanalysis to their regional air quality simulations over Europe with the WRF-CAMx mode.l The main objective of this work is the study of the impact of windblown dust, sea-salt aerosol and biogenic emissions on particle pollution levels in Europe using the novel natural emissions model (NEMO). Air quality simulations were performed for different emission scenarios in order to study the contribution of each natural emission source individually and together to air quality levels in Europe. The exclusion of windblown dust emissions decreases the mean seasonal PM10 levels by more than 3.3 mg/m^3 (~20%) in the Eastern Mediterranean during winter while an impact of 3 mg/m3 was also found during summer. The results also suggest that sea-salt aerosol has a significant effect on PM levels and composition (Figure 2).

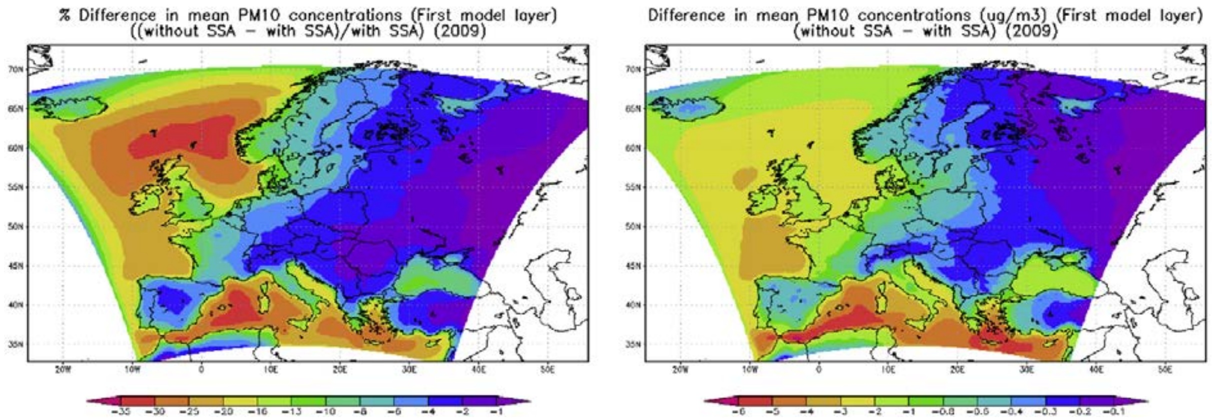

Figure 2: Mean annual percentage contribution (in %) of sea-salt aerosol (SSA) to PM10 levels (left) and mean annual impact of SSA on PM10 levels (in mg/m^3) (right) for 2009.

The MACC reanalysis data is evaluated by means of cluster analysis of European surface ozone observations in a recent paper by Lyapina et al. (2016). In their work, the regional representativeness of European ozone measurements is examined through a cluster analysis of 4 years of 3-hourly ozone data from 1492 European surface monitoring stations in the Airbase database. The individual clusters reveal differences in seasonal–diurnal cycles, showing typical patterns of the ozone behaviour for more polluted stations or more rural background. The seasonal, diurnal, and weekly cycles of each cluster are then compared to the MACC reanalysis. While the MACC reanalysis generally captures the shape of the diurnal cycles and the diurnal amplitudes, it is not able to reproduce the seasonal cycles very well and it exhibits a high bias up to 12 nmol mol^{-1} with a bias decreasing from more polluted clusters to cleaner ones. More generally, it can be shown that relatively coarse-scale global models are more suitable for simulation of regional background concentrations, which are less variable in space and time.

Other studies performed with ECMWF data products

In 2015 we started to use historical operational meteorological data and data from the ERA-INTERIM reanalysis to study the impact of meteorological data products on Lagrangian transport simulations of volcanic sulphur dioxide emissions (Hoffmann et al., 2016). We applied our new Lagrangian transport model Massive-Parallel Trajectory Calculations (MPTRAC) to perform simulations for three case studies of large volcanic eruption events in 2011. Besides validation of the new model, the main goal of the study was a comparison of the simulations with the different meteorological data products ERA-INTERIM, MERRA, and NCEP reanalyses, as well as ECMWF operational analyses. During the first 5 or 10 days after the eruptions we found the best performance for the ECMWF analysis by means of the Critical Success Index (CSI) (range of 0.25–0.31), followed by ERA-Interim (0.25–0.29), MERRA (0.23–0.27), and NCAR/NCEP (0.21–0.23). High temporal and spatial resolution of the meteorological data does lead to improved performance of Lagrangian transport simulations of volcanic emissions in the upper troposphere and lower stratosphere (Figure 3).

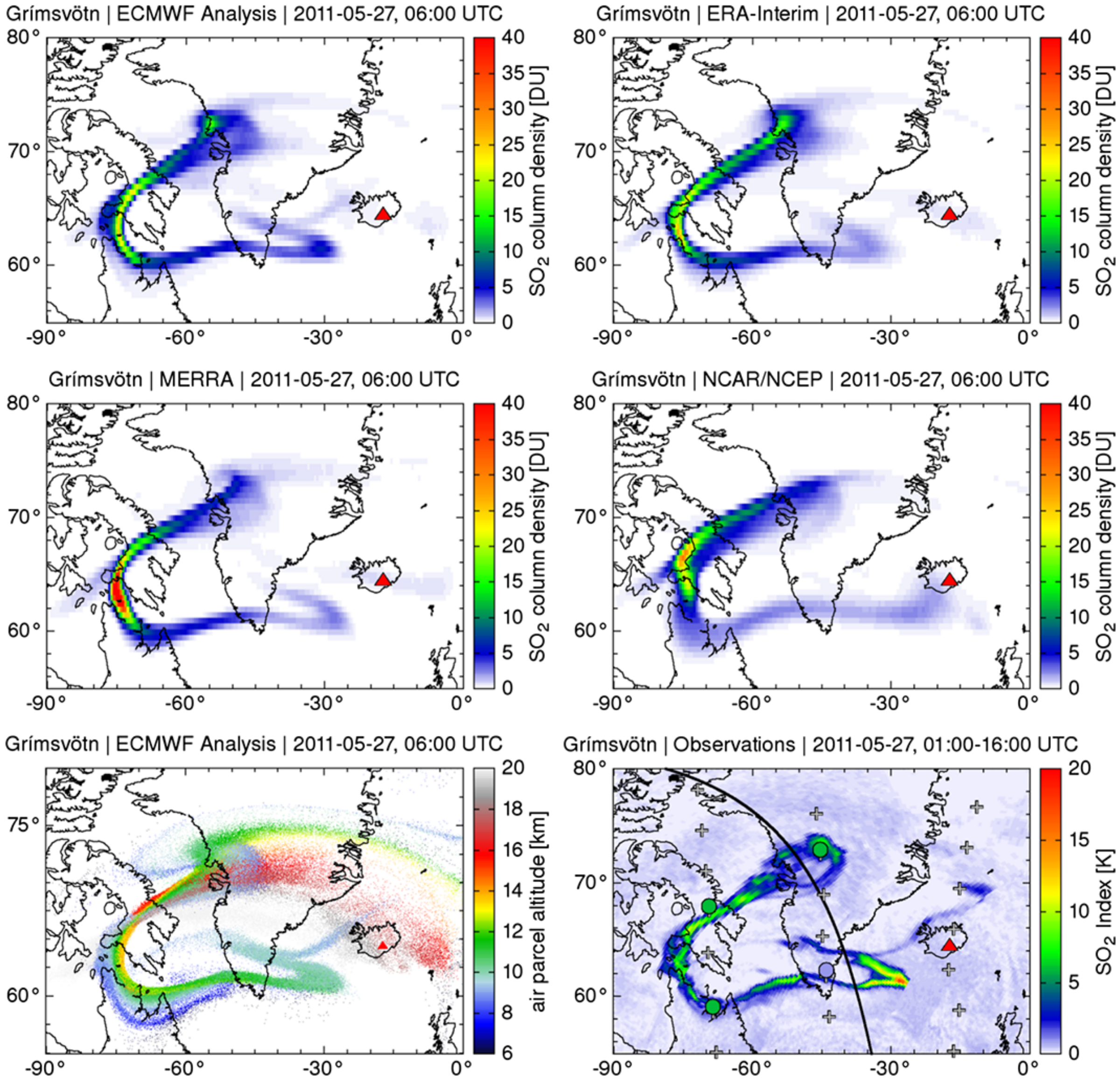

Figure 3: SO_2 column densities (top and middle rows) and air parcel altitudes (bottom, left) from Lagrangian transport simulations about 5 days after the eruption of Grímsvötn, Greenland in May 2011. Simulations are based on the same initialization, but make use of different meteorological data products. (bottom, right) A map of the AIRS SO_2 index (contour surface), MIPAS aerosol detections (circles), and a CALIPSO track (black line) are also shown. Color-coding indicates tangent altitudes of MIPAS aerosol detections (see bottom, left plot for color scale). Grey plus signs show MIPAS profiles without aerosol detections.

In a further study by Heng et al. (2016) we performed inverse transport modelling of volcanic sulphur dioxide emissions using large-scale simulations. The approach is based on the concepts of sequential importance resampling and parallel computing in order to reconstruct altitude-resolved time series of volcanic emissions, which often cannot be obtained directly with current measurement techniques. In the inverse modelling system MPTRAC is used to perform two types of simulations, i.e., unit simulations for the reconstruction of volcanic emissions and final forward simulations. Both types of transport simulations are based on wind fields of the ERA-Interim meteorological reanalysis. By using the critical success index (CSI), the simulation results are evaluated with AIRS observations. Compared to the results with an assumption of a constant flux of SO_2 emissions, our inversion approach leads to an improvement of the mean CSI value from 8.1 to 21.4 % and the maximum CSI value from 32.3 to 52.4 %. The simulation results are also compared with those reported in other studies and good agreement is observed.

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